

4-Hydroxy-1-naphthalenesulfonic acid monosodium salt
6099-57-6 | DTXSID6064113

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 332 °C

Global applicability domain: Outside

Local applicability domain index: 1.56e-01

Confidence level: 4.84e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Trimellitic anhydride

Measured: 390

Predicted: 366

[Image not found](#)

Benzoic acid, 2-benzoyl-

Measured: 261

Predicted: 309

[Image not found](#)

Benzoic acid, 2-phenoxy-

Measured: 355

Predicted: 325

[Image not found](#)

Benzoic acid, 2,4,5-trimethoxy-

Measured: 300

Predicted: 302